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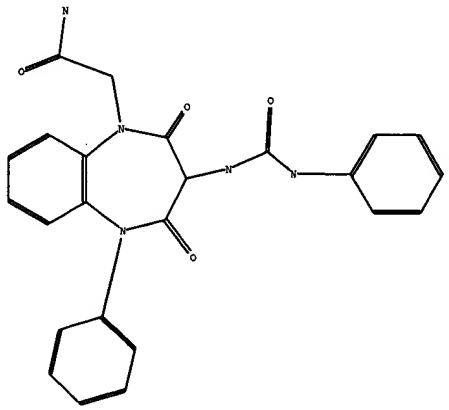

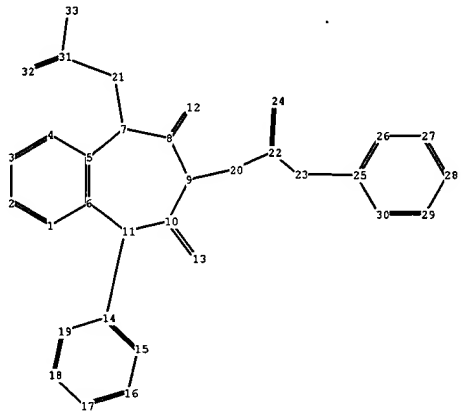

chain nodes :
12 13 20 21 22 23 24 31 32 33
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 14 15 16 17 18 19 25 26 27 28 29 30
chain bonds :
7-21 8-12 9-20 10-13 11-14 20-22 21-31 22-23 22-24 23-25 31-32 31-33
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-11 7-8 8-9 9-10 10-11 14-15 14-19 15-16 16-17 17-18 18-19 25-26 25-30 26-27 27-28 28-29 29-30
exact/norm bonds :
5-7 6-11 7-8 7-21 8-9 8-12 9-10 9-20 10-11 10-13 11-14 20-22 22-23 22-24 23-25 31-32 31-33
exact bonds :
21-31
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-19 15-16 16-17 17-18 18-19 25-26 25-30 26-27 27-28 28-29 29-30

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS

```
=> d his

     (FILE 'HOME' ENTERED AT 19:03:21 ON 31 JAN 2003)

     FILE 'REGISTRY' ENTERED AT 19:03:26 ON 31 JAN 2003
L1               STRUCTURE UPLOADED
L2               QUE L1
L3            14 S L2
L4           402 S L2 SSS FUL

     FILE 'CAPLUS' ENTERED AT 19:05:48 ON 31 JAN 2003
L5            49 S L4

     FILE 'REGISTRY' ENTERED AT 19:06:17 ON 31 JAN 2003
L6               STRUCTURE UPLOADED
L7               QUE L6
L8             9 S L7
L9           208 S L7  SUB=L4 FUL

     FILE 'CAPLUS' ENTERED AT 19:06:57 ON 31 JAN 2003
L10            34 S L9
L11          ANALYZE L10 1- RN HIT :     247 TERMS

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L12             1 S 151386-96-8/RN
L13               STRUCTURE UPLOADED
L14               QUE L13
L15             0 S L14  SUB=L4 SAM
L16            71 S L14  SUB=L4 FUL

     FILE 'CAPLUS' ENTERED AT 19:09:37 ON 31 JAN 2003
L17             9 S L16

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L2 HAS NO ANSWERS
L1               STR
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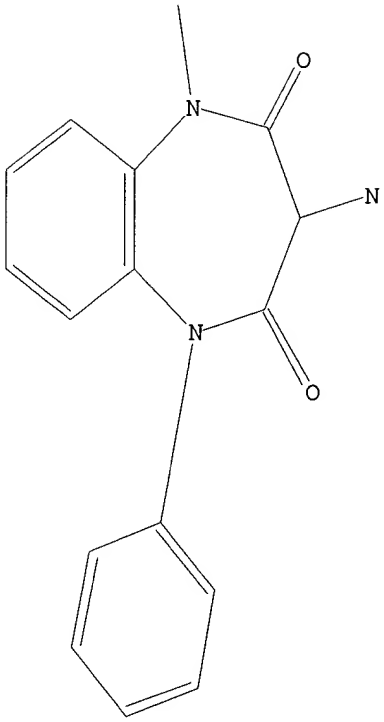
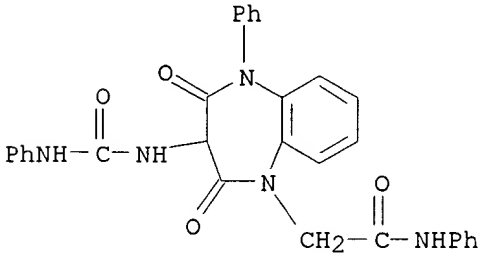


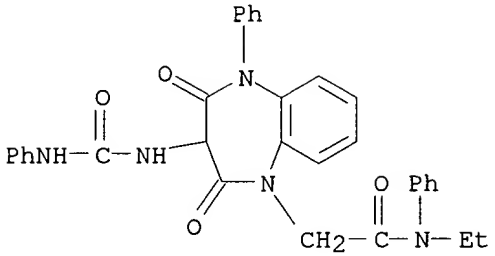

Structure attributes must be viewed using STN Express query preparation.
L2 QUE ABB=ON PLU=ON L1

=> d bib abs hitstr 1-9

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 2001:168978 CAPLUS
DN 134:335989
TI Nonpeptide cholecystokinin-2 receptor agonists
AU Kalindjian, S. Barret; Dunstone, David J.; Low, Caroline M. R.; Pether, Michael J.; Roberts, Sonia P.; Tozer, Matthew J.; Watt, Gillian F.; Shankley, Nigel P.
CS James Black Foundation, London, SE24 9JE, UK
SO Journal of Medicinal Chemistry (2001), 44(8), 1125-1133
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB In the course of structural explorations around a series of potent CCK2 receptor antagonists, it was noted that simple N-methylation of the indolic N-H in the parent mol. gave rise to behavior in vivo that was consistent with the compd. acting as an agonist. Exploration in vitro confirmed this property, and it was shown that the agonist action could be blocked by the ref. CCK2 receptor antagonist, L-365,260. Further examples of this type of modification were explored, and a common theme with regard to agonist behavior was uncovered. Some mol. modeling is also presented in an attempt to throw light on the nature of the ligand receptor interactions that may be giving rise to the differing properties of these, apparently, structurally similar mols.
IT **173908-65-1P 173908-67-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(structure-activity relationship of nonpeptide cholecystokinin-2 receptor agonists)
RN 173908-65-1 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)




RN 173908-67-3 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-ethyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

applicant

L17 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 2000:814470 CAPLUS
DN 133:350255
TI Preparation of 1,5-benzodiazepine derivatives as CCK-A receptor agonists
IN Colclough, David; Hodgson, Anne; Szewczyk, Jerzy Ryszard
PA Glaxo Group Ltd., UK
SO PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2000068209 | A2 | 20001116 | WO 2000-EP3982 | 20000504 |
| | WO 2000068209 | A3 | 20010301 | | |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | BR 2000010338 | A | 20020213 | BR 2000-10338 | 20000504 |
| | EP 1212305 | A2 | 20020612 | EP 2000-929488 | 20000504 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| | JP 2002544200 | T2 | 20021224 | JP 2000-617189 | 20000504 |
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| PRAI | GB 1999-10366 | A | 19990506 | | |
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| | WO 2000-EP3982 | W | 20000504 | | |

OS MARPAT 133:350255
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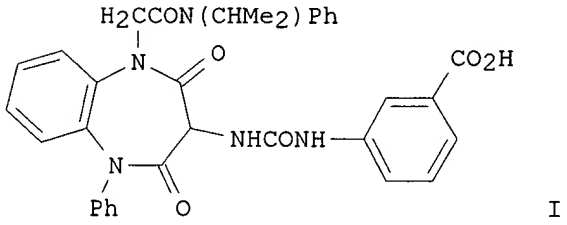



I

AB An enantiomerically enriched 1,5-benzodiazepine compd. I is disclosed. Use of I for the treatment of CCK-A mediated diseases or conditions, such as obesity, is indicated.

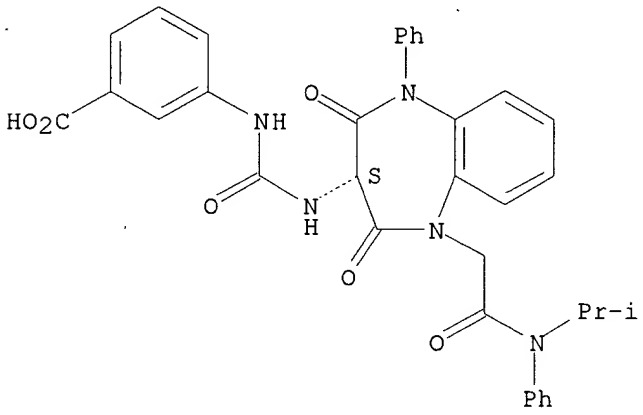
IT **305366-98-7P 305366-99-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 1,5-benzodiazepine derivs. as CCK-A receptor agonists)

RN 305366-98-7 CAPLUS

CN Benzoic acid, 3-[[[[(3S)-2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

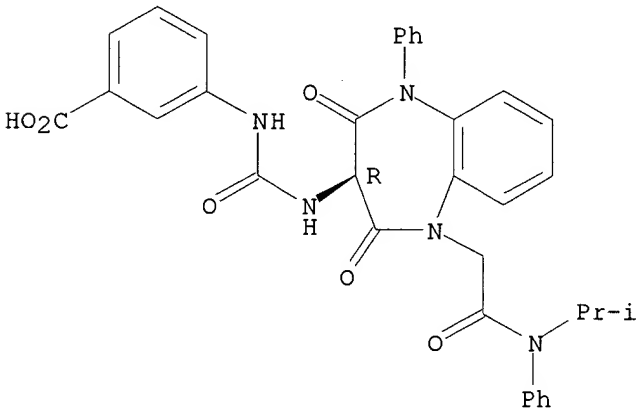
Absolute stereochemistry. Rotation (+).



RN 305366-99-8 CAPLUS

CN Benzoic acid, 3-[[[[(3R)-2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **305366-94-3P**

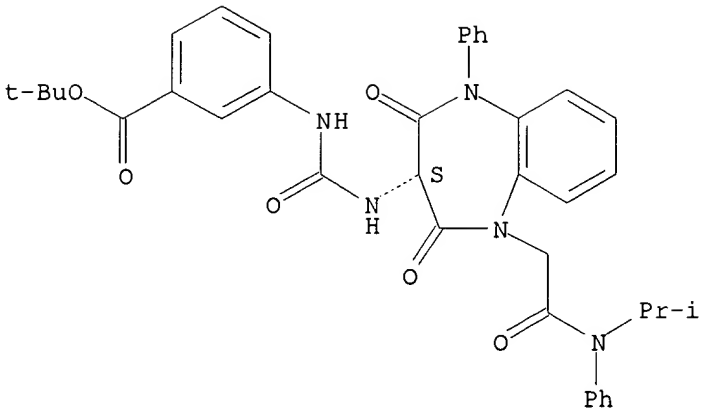
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 1,5-benzodiazepine derivs. as CCK-A receptor agonists)

RN 305366-94-3 CAPLUS

CN Benzoic acid, 3-[[[[(3S)-2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).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NH
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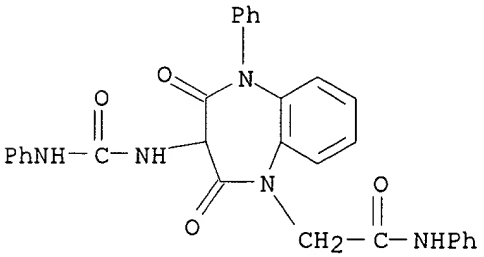
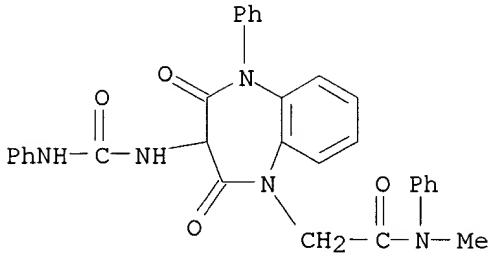
N
Ph

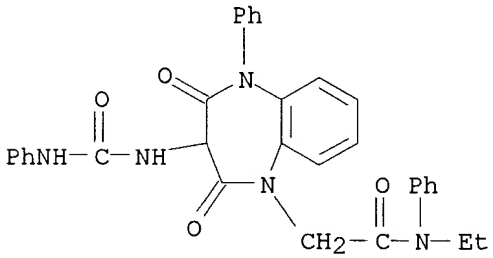
L10 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 2000:391139 CAPLUS
DN 133:129526
TI Computer prediction of biological activity spectra for low-molecular peptides and peptidomimetics
AU Martynova, N. B.; Filimonov, D. A.; Poroikov, V. V.
CS Institute of Biomedical Chemistry, Russian Academy of Medical Sciences, Moscow, 119832, Russia
SO Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya) (2000), 26(5), 297-305
CODEN: RJBCET; ISSN: 1068-1620
PB MAIK Nauka/Interperiodica
DT Journal
LA English
AB The wide variety of the biol. effects of peptides and their high activity are the main reasons for the search for new basic drug structures among them. The most promising compds. can be selected using the PASS computer system (Prediction of Activity Spectra for Substances). This system was originally developed to predict the activities of low-mol. "drug-like" org. compds. Its predictive capacity is described here by the example of 134 peptides and peptidomimetics with nine known biol. activities. Its av. predictive power is shown to be approx. 97%. Such an accuracy demonstrates that computer prediction can be applied both to the evaluation of effects and mechanisms of action of endogenous and synthetic peptides and to the screening of new therapeutic agents among the most promising basic structures.
IT **173908-65-1 173908-66-2 173908-67-3**
**173908-68-4 173908-69-5 173908-70-8**
**173908-71-9 173908-72-0 173908-73-1**
**173908-75-3 173908-76-4 173908-77-5**
**173908-78-6 173908-79-7 173908-82-2**
**173908-83-3 173908-84-4 173908-85-5**
**173908-86-6 173908-87-7**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(cholecystokinin receptor agonist; computer prediction of biol. activity spectra for low-mol. peptides and peptidomimetics)
RN 173908-65-1 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



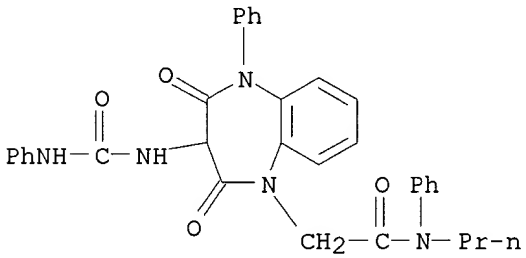

RN 173908-66-2 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-methyl-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



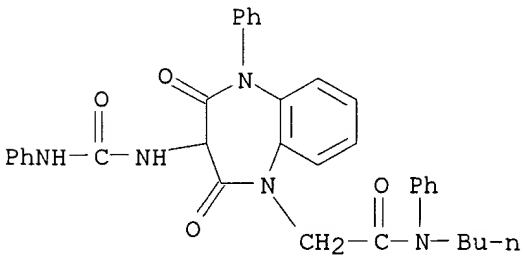
RN 173908-67-3 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-ethyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



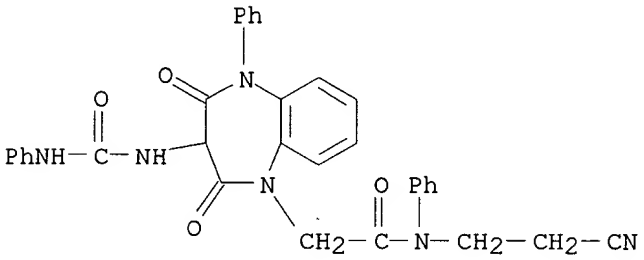
RN 173908-68-4 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]-N-propyl- (9CI) (CA INDEX NAME)



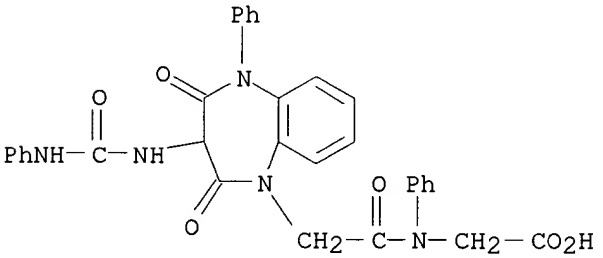
RN 173908-69-5 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-butyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



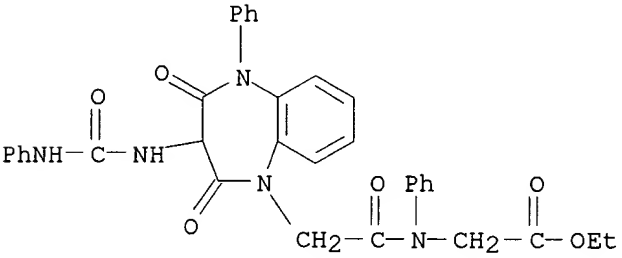
RN 173908-70-8 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-(2-cyanoethyl)-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



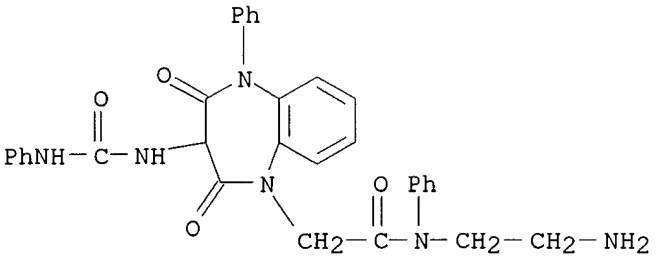
RN 173908-71-9 CAPLUS
CN Glycine, N-phenyl-N-[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-1H-1,5-benzodiazepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)



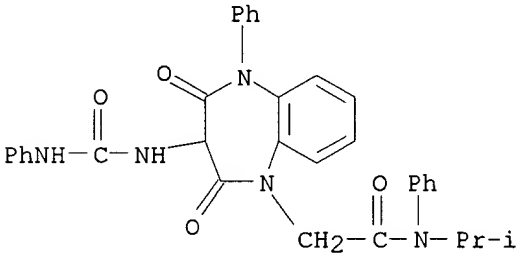
RN 173908-72-0 CAPLUS
CN Glycine, N-phenyl-N-[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-1H-1,5-benzodiazepin-1-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)



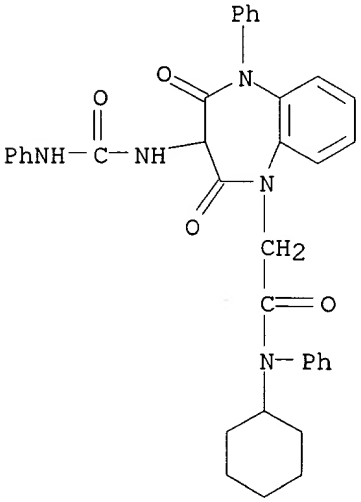
RN 173908-73-1 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-(2-aminoethyl)-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



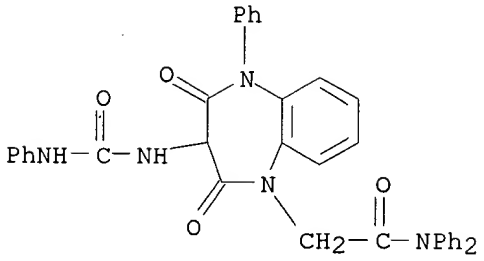
RN 173908-75-3 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



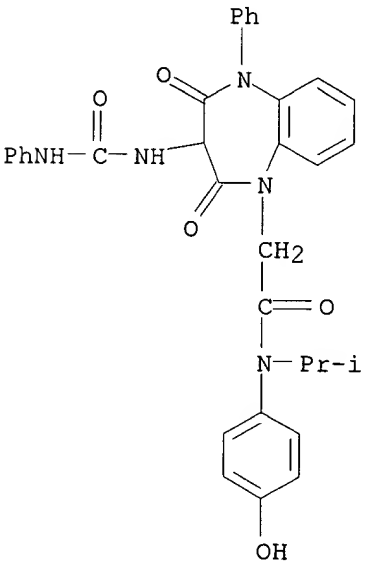
RN 173908-76-4 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-cyclohexyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 173908-77-5 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,N,5-triphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 173908-78-6 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(4-hydroxyphenyl)-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-(9CI) (CA INDEX NAME)



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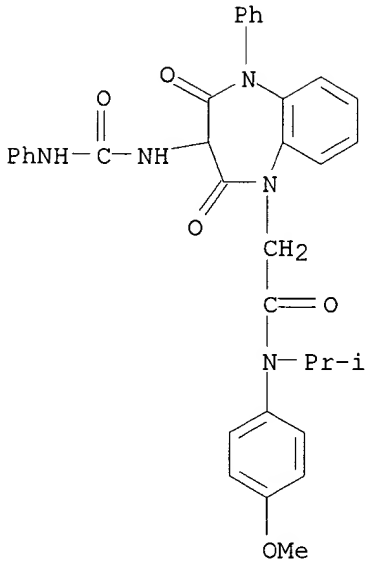
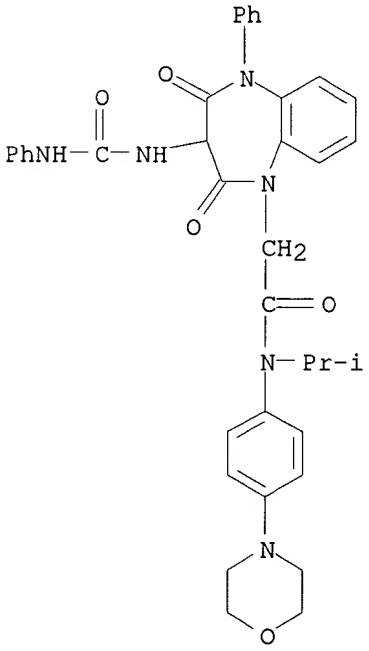
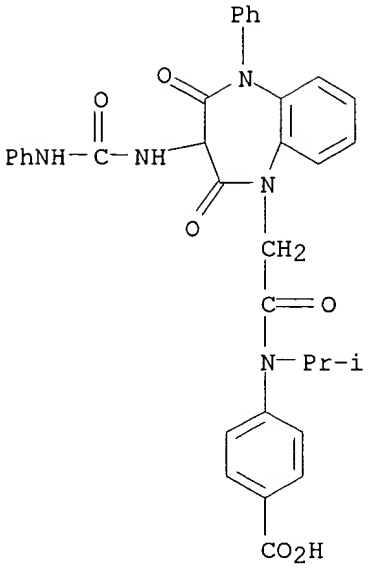
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(4-methoxyphenyl)-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-(9CI) (CA INDEX NAME)



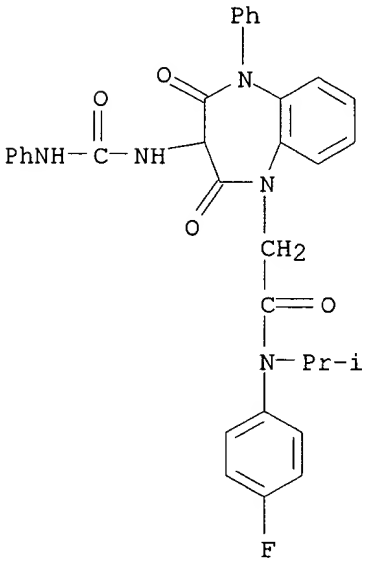
RN 173908-82-2 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-N-[4-(4-morpholinyl)phenyl]-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



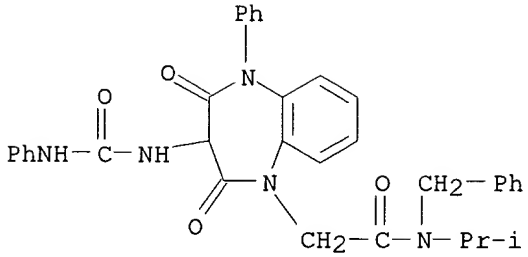
RN 173908-83-3 CAPLUS
CN Benzoic acid, 4-[(1-methylethyl)[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-1H-1,5-benzodiazepin-1-yl]acetyl]amino]- (9CI) (CA INDEX NAME)



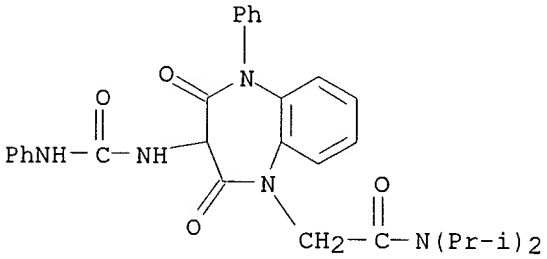
RN 173908-84-4 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-(4-fluorophenyl)-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



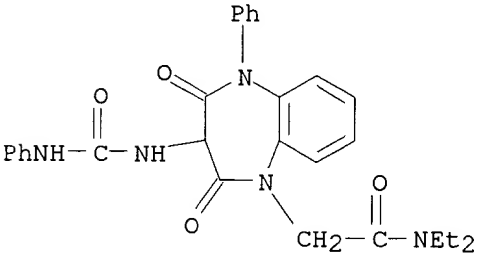
RN 173908-85-5 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 173908-86-6 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N,N-bis(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)

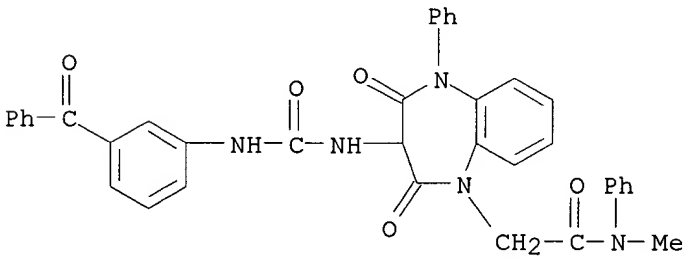


RN 173908-87-7 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N,N-diethyl-2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)

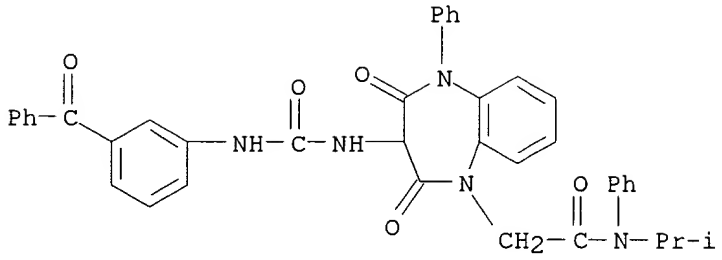


RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

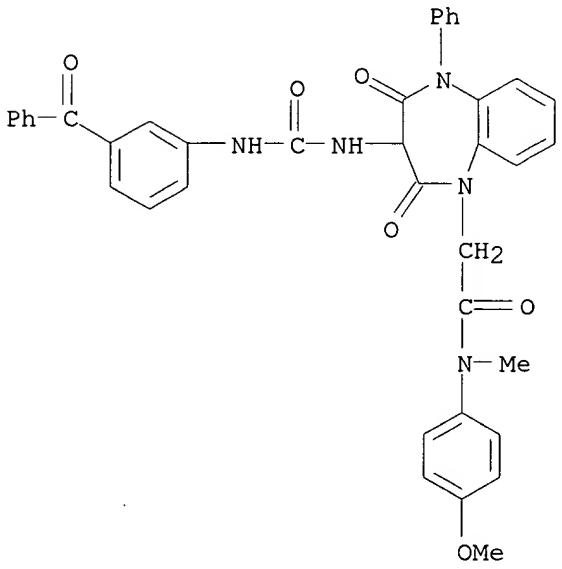
L17 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1999:1261 CAPLUS
DN 130:163293
TI Structurally similar small molecule photoaffinity CCK-A agonists and antagonists as novel tools for directly probing 7TM receptor-ligand interactions
AU Darrow, James W.; Hadac, Elizabeth M.; Miller, Laurence J.; Sugg, Elizabeth E.
CS Neurogen Corporation, Branford, CT, 06405, USA
SO Bioorganic & Medicinal Chemistry Letters (1998), 8(22), 3127-3132
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
AB Incorporation of photolabile benzoyl (2a-d) or trifluoromethyl-3H-diazirine (3a-d) substituents into 1,5-benzodiazepine ligands did not significantly impair the rat CCK-A binding affinity of either agonists or antagonists. The modified agonist ligands also retained functional potency and efficacy in the rat amylase assay. Despite their strong structural similarity, the SAR of this limited set of compds. suggests that these small mol. antagonists and agonists might differ in their mode of binding to the CCK-A receptor. Preliminary affinity results show that representative agonists and antagonists from these series can be used to efficiently covalently label the CCK-A receptor.
IT **220493-38-9P 220493-39-0P 220493-40-3P**
**220493-41-4P 220493-42-5P 220493-43-6P**
**220493-44-7P 220493-45-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PNU (Preparation, unclassified); BIOL (Biological study); PREP (Preparation)
(affinity of, to bind CCK-A receptor,; incorporation of photolabile benzoyl or trifluoromethyl-3H-diazirine substituents into benzodiazepine ligands)
RN 220493-38-9 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-benzoylphenyl)amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-methyl-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



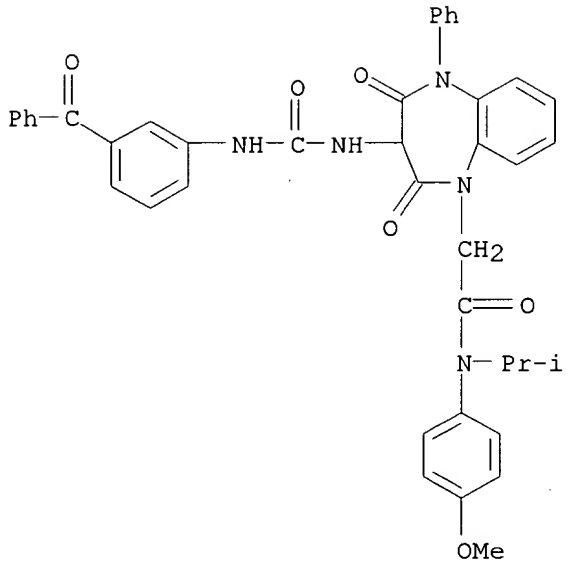
RN 220493-39-0 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-benzoylphenyl)amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



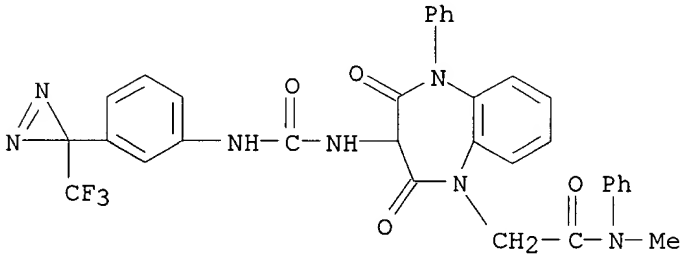
RN 220493-40-3 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-benzoylphenyl)amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(4-methoxyphenyl)-N-methyl-2,4-dioxo-5-phenyl- (9CI) (CA INDEX NAME)



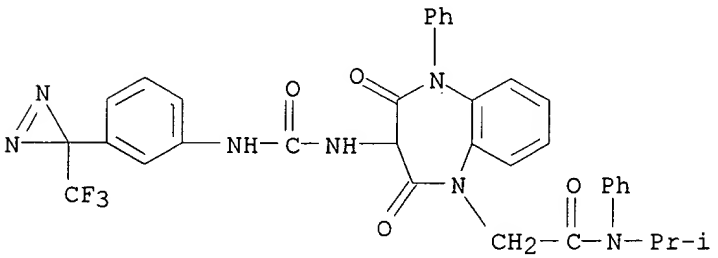
RN 220493-41-4 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-benzoylphenyl)amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(4-methoxyphenyl)-N-(1-methylethyl)-2,4-dioxo-5-phenyl- (9CI) (CA INDEX NAME)



RN 220493-42-5 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-methyl-2,4-dioxo-N,5-diphenyl-3-[[[[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

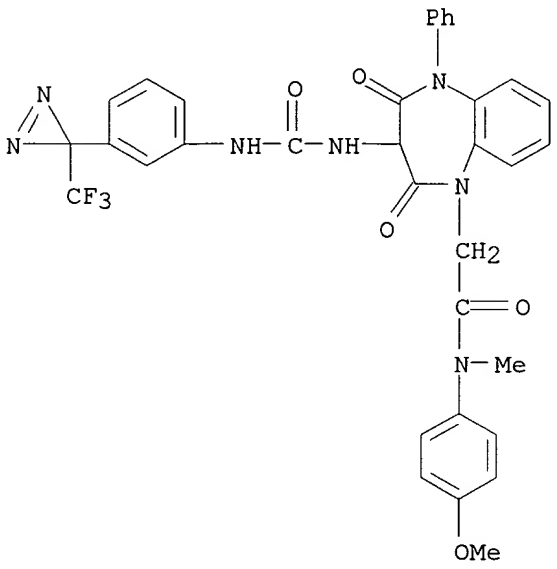


RN 220493-43-6 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[[[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



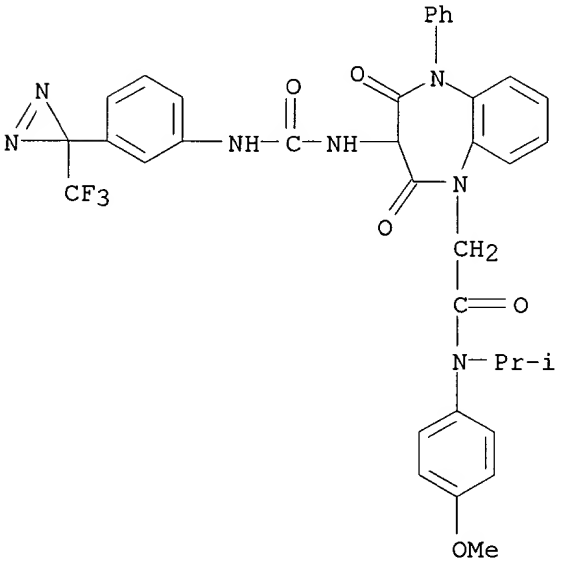
RN 220493-44-7 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(4-methoxyphenyl)-N-methyl-2,4-dioxo-5-phenyl-3-[[[[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



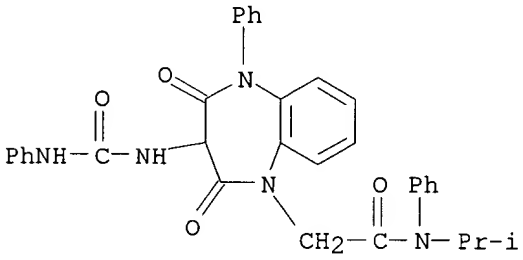
RN 220493-45-8 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(4-methoxyphenyl)-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[[[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

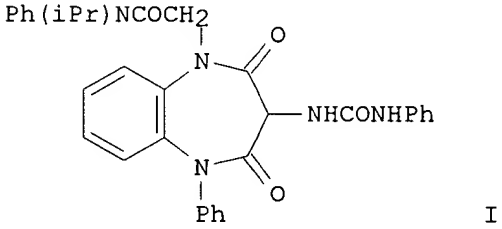


RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1997:188924 CAPLUS
DN 126:271812
TI Conversion of acyclic nonpeptide CCK antagonists into CCK agonists
AU Hirst, Gavin C.; Queen, Kennedy L.; Sugg, Elizabeth E.; Willson, Timothy M.
CS Department of Medicinal Chemistry, Glaxo Wellcome Research and Development, Research Triangle Park, NC, 27709, USA
SO Bioorganic & Medicinal Chemistry Letters (1997), 7(5), 511-514
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier
DT Journal
LA English
OS CASREACT 126:271812
AB The CCK antagonists RP 69758 and (R)-lorglumide were converted into CCK agonists by the introduction of an N-isopropylanilide agonist "trigger.". The common structural features of these ligands suggest that nonpeptide agonists and antagonists bind to a common site in the CCK receptor.
IT **173908-75-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(conversion of acyclic nonpeptide cholecystokinin antagonists into cholecystokinin agonists by structural modification)
RN 173908-75-3 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



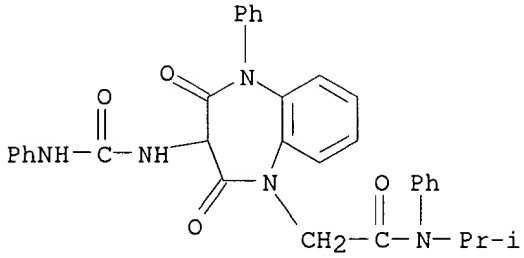
L17 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1996:713053 CAPLUS
DN 126:42245
TI Discovery of 1,5-Benzodiazepines with Peripheral Cholecystokinin (CCK-A) Receptor Agonist Activity (II): Optimization of the C3 Amino Substituent
AU Hirst, Gavin C.; Aquino, Christopher; Birkemo, Lawrence; Croom, Dallas K.; Dezube, Milana; Dougherty, Robert W., Jr.; Ervin, Gregory N.; Grizzle, Mary K.; Hanke, Brad; et al.
CS Department of Medicinal Chemistry, Glaxo Wellcome Research and Development, Research Triangle Park, NC, 27709, USA
SO Journal of Medicinal Chemistry (1996), 39(26), 5236-5245
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI




I

AB Analogs of the previously reported 1,5-benzodiazepine peripheral cholecystokinin (CCK-A) receptor agonist (I) were prepd. which explore substitution and/or replacement of the C-3 Ph urea moiety. Agonist efficacy on the isolated guinea pig gallbladder (GPGB) was retained with a variety of substituted ureas and amide analogs. Three compds. were identified which were orally active in the mouse gallbladder emptying assay (MGBE). The 2-indolamide and N-(carboxymethyl)-2-indolamide derivs. had improved affinity for the human CCK-A receptor but reduced agonist efficacy on the GPGB. Neither indolamide was orally active in a rat feeding assay. In contrast, the (3-carboxyphenyl)urea deriv. (GW7854) had moderately increased affinity for the human CCK-B receptor but was a potent full agonist on the GPGB and was orally active in both the MGBE and rat feeding assays. GW7854 was a full agonist (EC50 = 60 nM) for calcium mobilization on CHO K1 cells expressing hCCK-A receptors and a potent antagonist of CCK-8 (pA2 = 9.1) on CHO K1 cells expressing hCCK-B receptors. GW7854 is a potent mixed CCK-A agonist/CCK-B antagonist which is orally active in two in vivo models of CCK-A-mediated agonist activity.

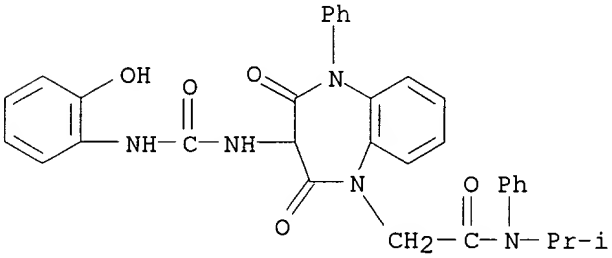
IT **173908-75-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(prepn. and structure activity relations of 1,5-benzodiazepines as peripheral cholecystokinin (CCK-A) receptor agonists)
RN 173908-75-3 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



IT **184944-94-3P 184944-95-4P 184944-96-5P**
**184944-97-6P 184944-98-7P 184944-99-8P**
**184945-00-4P 184945-01-5P 184945-02-6P**
**184945-03-7P 184945-04-8P 184945-05-9P**
**184945-06-0P 184945-07-1P 184945-08-2P**
**184945-09-3P 184945-10-6P 184945-11-7P**
**184945-12-8P 184945-13-9P 184945-14-0P**
**184945-15-1P 184945-16-2P 184945-30-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and structure activity relations of 1,5-benzodiazepines as peripheral cholecystokinin (CCK-A) receptor agonists)

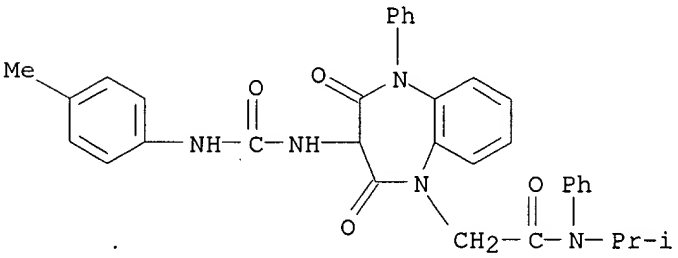
RN 184944-94-3 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-[[[(2-hydroxyphenyl)amino]carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)

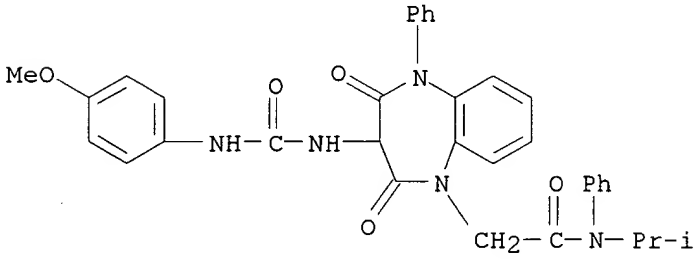


RN 184944-95-4 CAPLUS

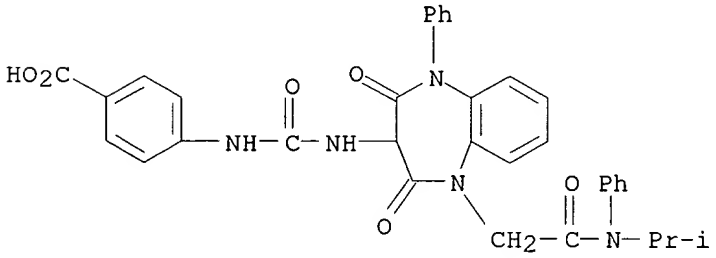
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[(4-methylphenyl)amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



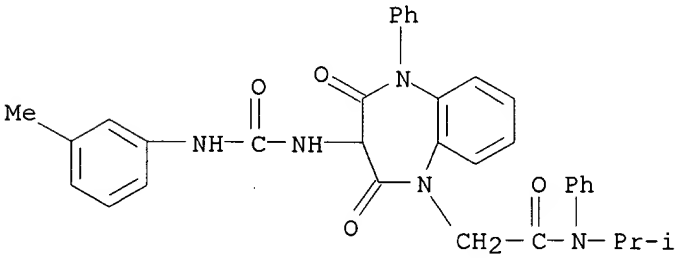
RN 184944-96-5 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-[[[(4-methoxyphenyl)amino]carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



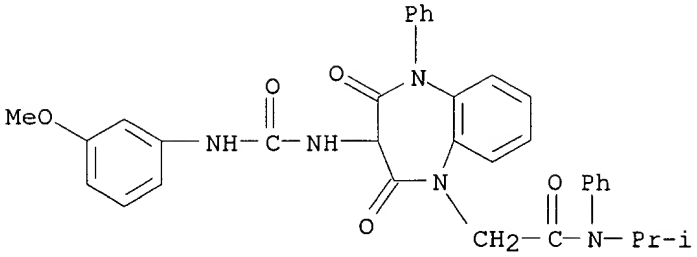
RN 184944-97-6 CAPLUS
CN Benzoic acid, 4-[[[[2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



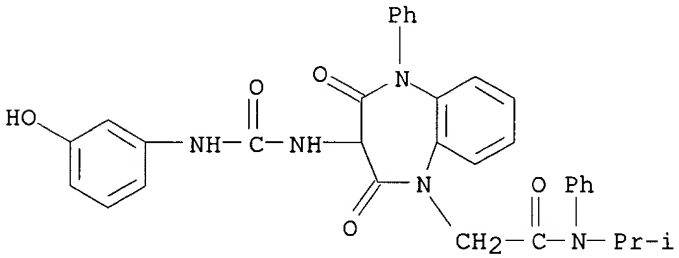
RN 184944-98-7 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[(3-methylphenyl)amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



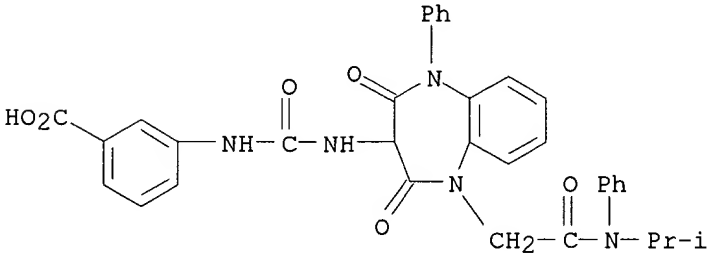
RN 184944-99-8 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-[[[(3-methoxyphenyl)amino]carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



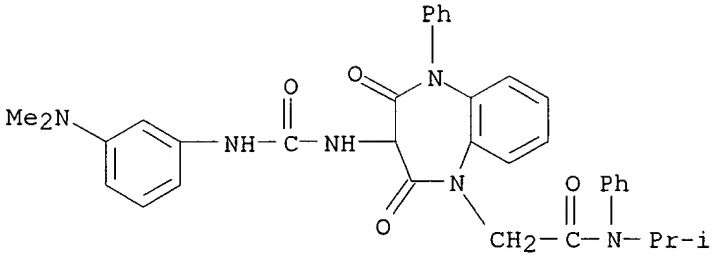
RN 184945-00-4 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-[[[(3-hydroxyphenyl)amino]carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



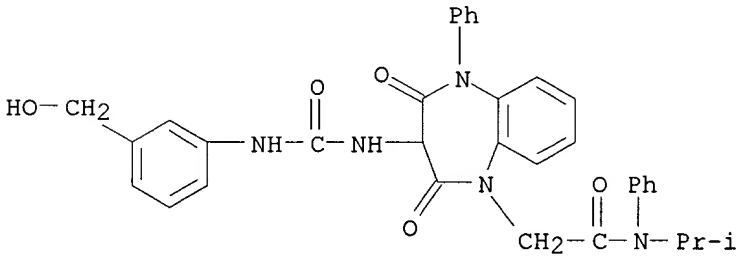
RN 184945-01-5 CAPLUS
CN Benzoic acid, 3-[[[[2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



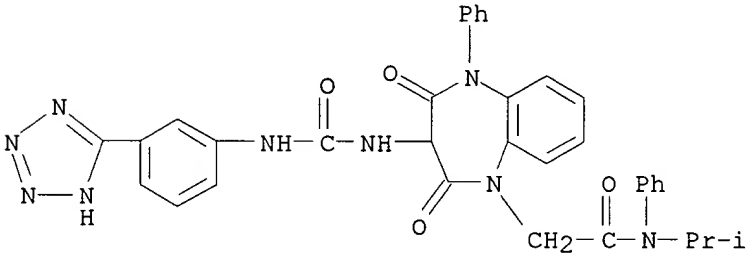
RN 184945-02-6 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[[3-(dimethylamino)phenyl]amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



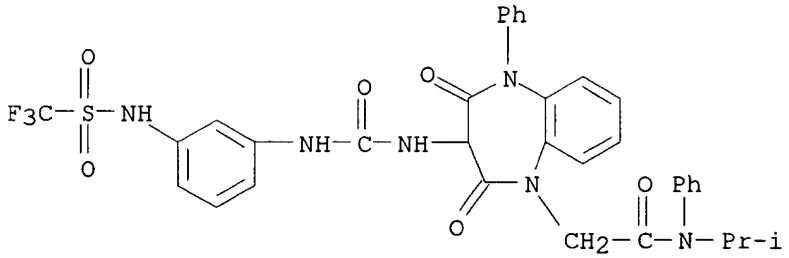
RN 184945-03-7 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-[[[[3-(hydroxymethyl)phenyl]amino]carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



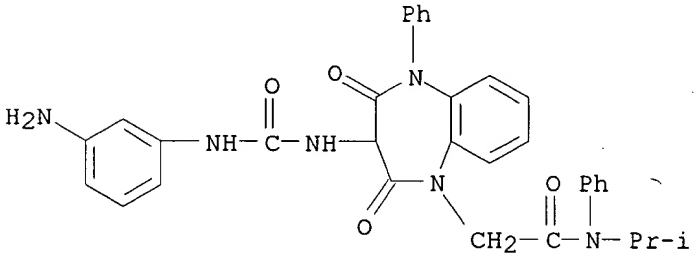
RN 184945-04-8 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[[[3-(1H-tetrazol-5-yl)phenyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



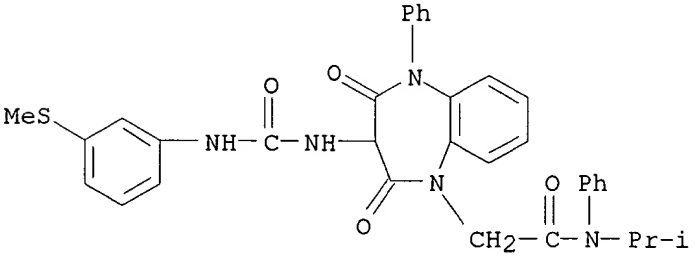
RN 184945-05-9 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[[[3-[[(trifluoromethyl)sulfonyl]amino]phenyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



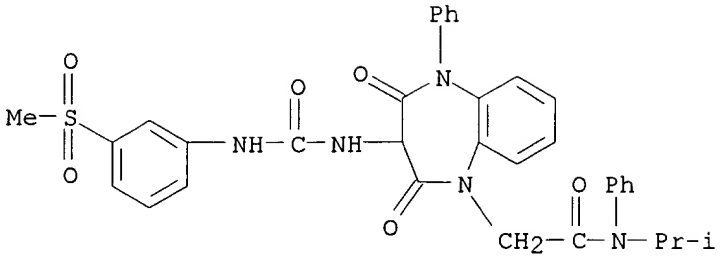
RN 184945-06-0 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-aminophenyl)amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



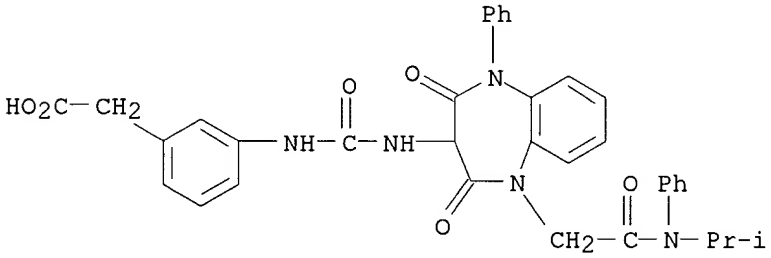
RN 184945-07-1 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[[3-(methylthio)phenyl]amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



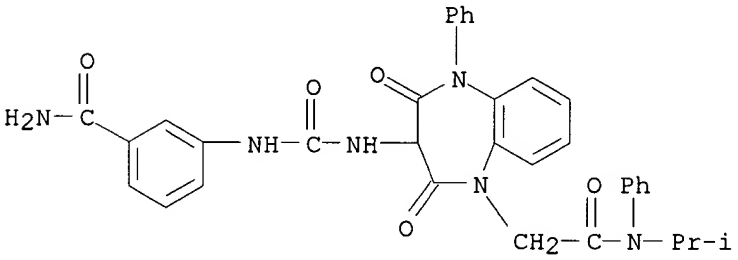
RN 184945-08-2 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[[3-(methylsulfonyl)phenyl]amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



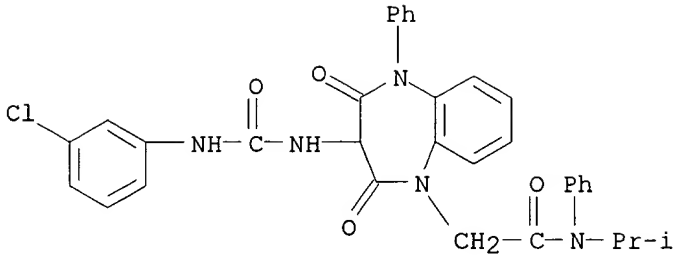
RN 184945-09-3 CAPLUS
CN Benzeneacetic acid, 3-[[[[2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



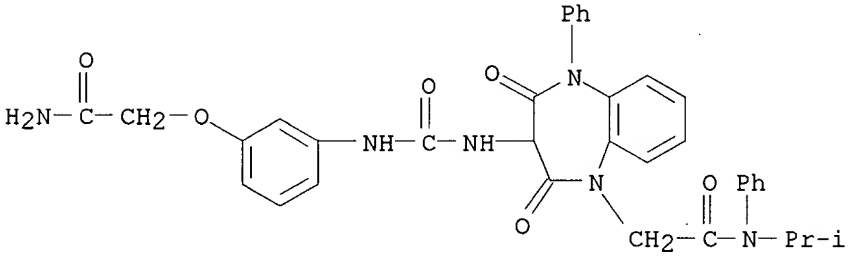
RN 184945-10-6 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[[3-(aminocarbonyl)phenyl]amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



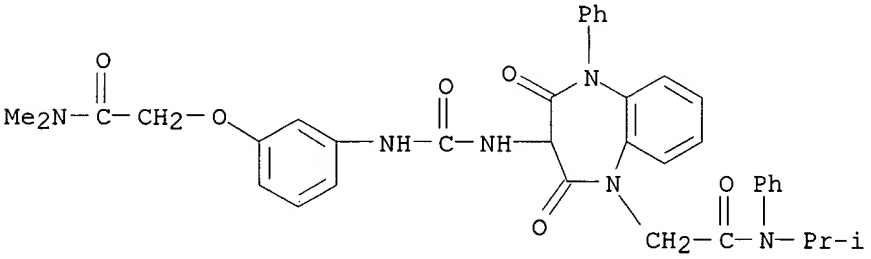
RN 184945-11-7 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-chlorophenyl)amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



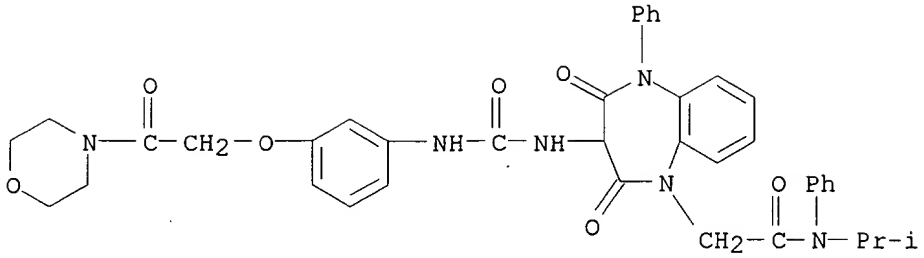
RN 184945-12-8 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[[3-(2-amino-2-oxoethoxy)phenyl]amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



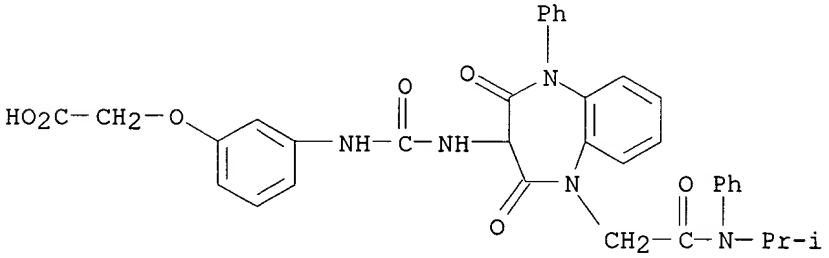
RN 184945-13-9 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[[3-[2-(dimethylamino)-2-oxoethoxy]phenyl]amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



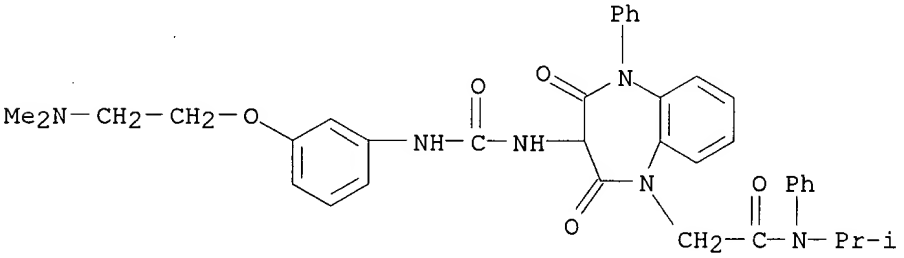
RN 184945-14-0 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[[3-[2-(4-morpholinyl)-2-oxoethoxy]phenyl]amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



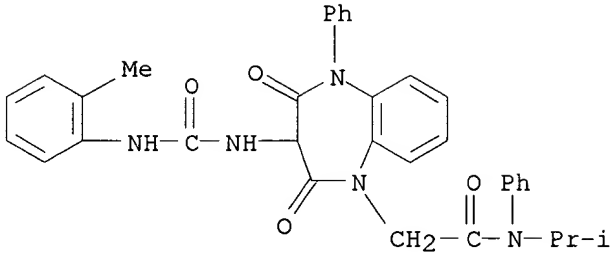
RN 184945-15-1 CAPLUS
CN Acetic acid, [3-[[[[2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]phenoxy]- (9CI) (CA INDEX NAME)



RN 184945-16-2 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[[3-[2-(dimethylamino)ethoxy]phenyl]amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



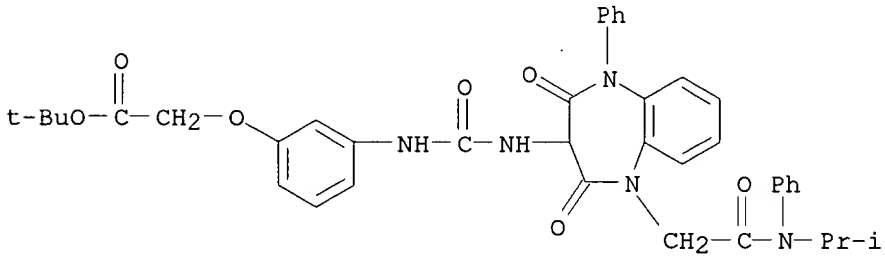
RN 184945-30-0 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[(2-methylphenyl)amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



IT **184944-89-6P 184945-28-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and structure activity relations of 1,5-benzodiazepines as peripheral cholecystokinin (CCK-A) receptor agonists)

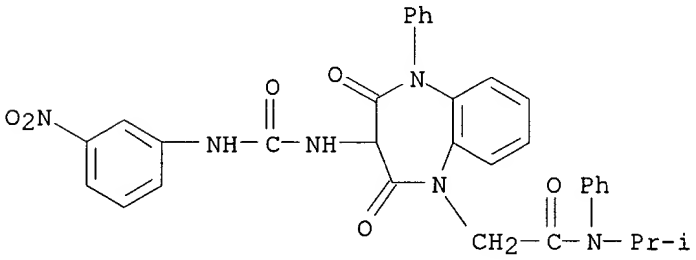
RN 184944-89-6 CAPLUS

CN Acetic acid, [3-[[[[2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]phenoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

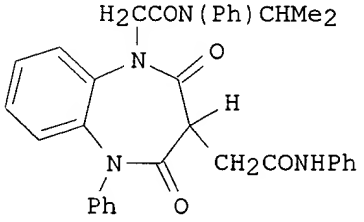


RN 184945-28-6 CAPLUS

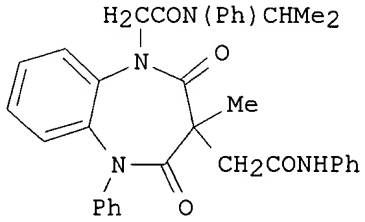
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[(3-nitrophenyl)amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



L17 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1996:382879 CAPLUS
DN 125:104231
TI 3-[2-(N-Phenylacetamide)]-1,5-benzodiazepines: Orally Active, Binding Selective CCK-A Agonists
AU Willson, Timothy M.; Henke, Brad R.; Momtahen, Tanya M.; Myers, Peter L.; Sugg, Elizabeth E.; Unwalla, Rayomand J.; Croom, Dallas K.; Dougherty, Robert W.; Grizzle, Mary K.; et al.
CS Glaxo Wellcome Research and Development, Research Triangle Park, NC, 27709, USA
SO Journal of Medicinal Chemistry (1996), 39(15), 3030-3034
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI




I

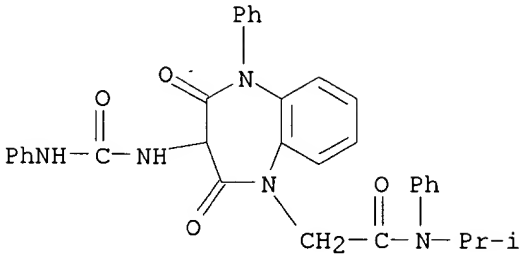



II

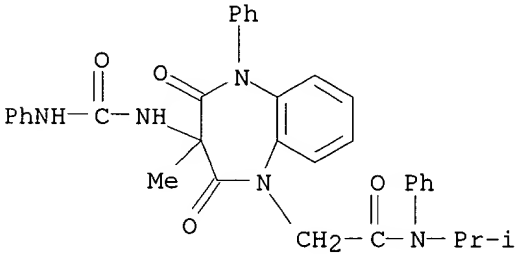
AB A series of modifications were made to the C-3 substituent of the 1,5-benzodiazepine CCK-A agonist I. Replacement of the inner urea NH and addn. of a Me group to generate a C-3 quaternary carbon resulted in acetamide II, which showed CCK-A receptor binding selectivity and sub-micromolar agonist activity in vitro. II was active in an in vivo mouse gallbladder emptying assay and represents a novel orally active, binding selective CCK-A agonist.

IT **173908-75-3P 178983-16-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-[2-(N-phenylacetamide)]-1,5-benzodiazepines as orally active, binding selective CCK-A agonists)

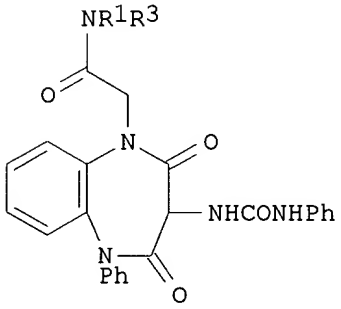
RN 173908-75-3 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 178983-16-9 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-methyl-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]-(9CI) (CA INDEX NAME)



L17 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1996:6885 CAPLUS
DN 124:176049
TI Discovery of 1,5-benzodiazepines with peripheral cholecystokinin (CCK-A) receptor agonist activity. 1. Optimization of the agonist "trigger"
AU Aquino, Christopher J.; Armour, Duncan R.; Berman, Judd M.; Birkemo, Larry S.; Carr, Robin A. E.; Croom, Dallas K.; Dezube, Milana; Dougherty, Robert W., Jr.; Ervin, Gregory N.; et al.
CS Department of Medicinal Chemistry, Glaxo Wellcome, Research Triangle Park, NC, 27709, USA
SO Journal of Medicinal Chemistry (1996), 39(2), 562-9
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI




I

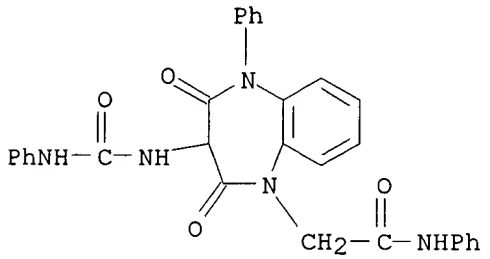
AB Directed screening of compds. selected from the Glaxo registry file for contractile activity on the isolated guinea pig gallbladder identified a series of 1,5-benzodiazepines [I; R1 = H, Me, Et, Pr, Bu, CH2CH2CN, CHMe2, cyclohexyl, Ph, etc.; R3 = (substituted) Ph, etc.] with peripheral cholecystokinin (CCK) receptor agonist activity. Agonist efficacy within this series was modulated by variation of substituents on the N1-anilinoacetamide moiety. Remarkably, a single Me group confers agonist activity, with a CHMe2 providing optimal efficacy. Hydrophilic substituents on the anilino N abolish agonist activity or produce antagonists of CCK. In contrast, hydrophilic electron-donating groups at the para-position of the anilino ring enhance or maintain in vitro and in vivo agonist activity. Despite decreased affinity for the human CCK-A receptor relative to CCK-8, some I are equipotent to CCK as anorectic agents in rats following i.p. administration.

IT **173908-65-1P 173908-66-2P 173908-67-3P**
**173908-68-4P 173908-69-5P 173908-70-8P**
**173908-71-9P 173908-72-0P 173908-73-1P**
**173908-74-2P 173908-75-3P 173908-76-4P**
**173908-77-5P 173908-78-6P 173908-79-7P**
**173908-81-1P 173908-82-2P 173908-83-3P**
**173908-84-4P 173908-85-5P 173908-86-6P**
**173908-87-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of 1,5-benzodiazepines with peripheral cholecystokinin (CCK-A)

agonist activity)

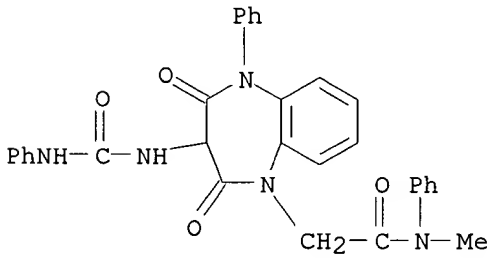
RN 173908-65-1 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



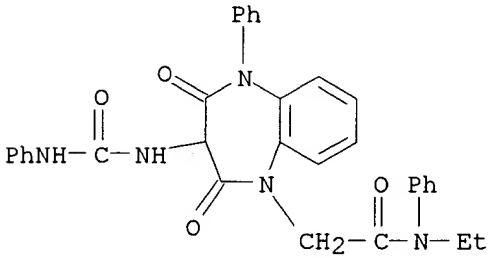
RN 173908-66-2 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-methyl-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



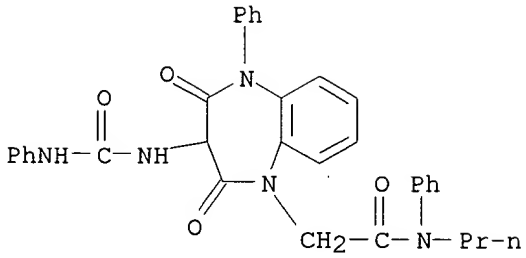
RN 173908-67-3 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, N-ethyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)

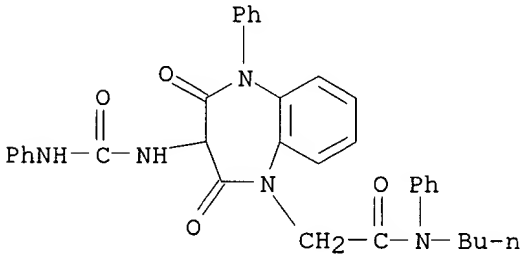


RN 173908-68-4 CAPLUS

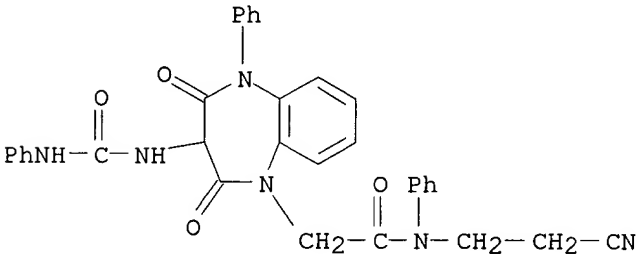
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]-N-propyl- (9CI) (CA INDEX NAME)



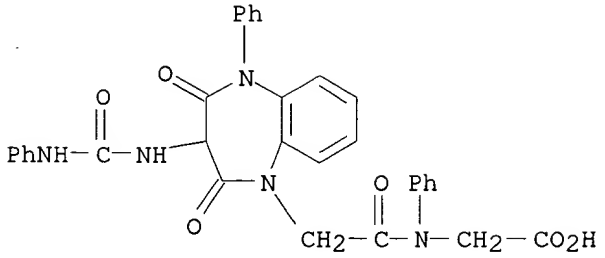
RN 173908-69-5 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-butyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



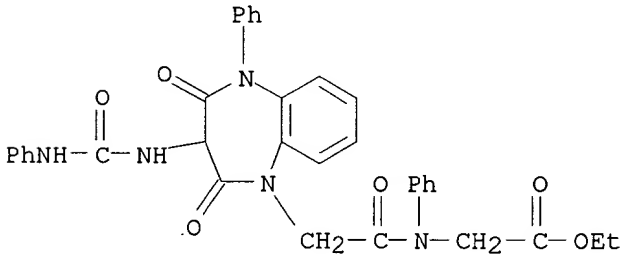
RN 173908-70-8 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-(2-cyanoethyl)-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



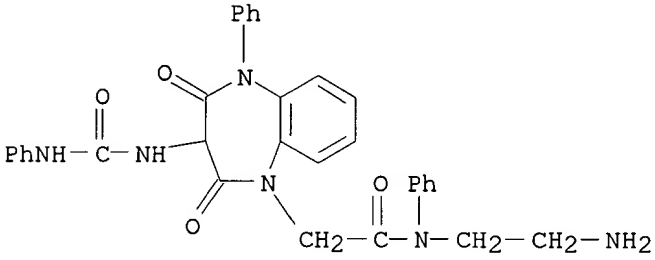
RN 173908-71-9 CAPLUS
CN Glycine, N-phenyl-N-[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-1H-1,5-benzodiazepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)



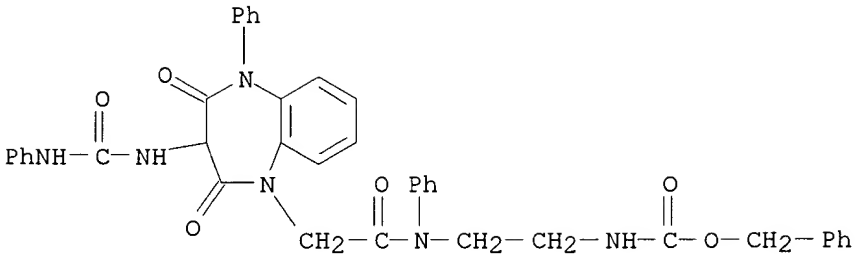
RN 173908-72-0 CAPLUS
CN Glycine, N-phenyl-N-[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-1H-1,5-benzodiazepin-1-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)



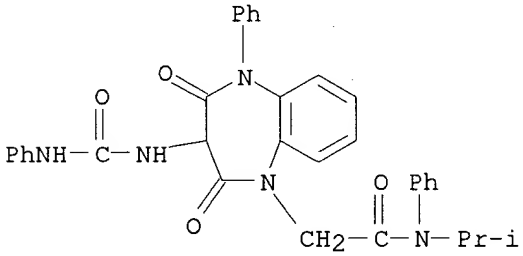
RN 173908-73-1 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-(2-aminoethyl)-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



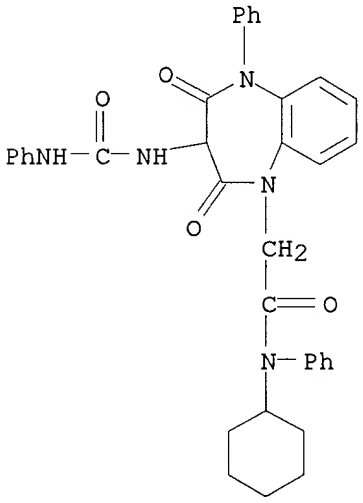
RN 173908-74-2 CAPLUS
CN Carbamic acid, [2-[phenyl[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-1H-1,5-benzodiazepin-1-yl]acetyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



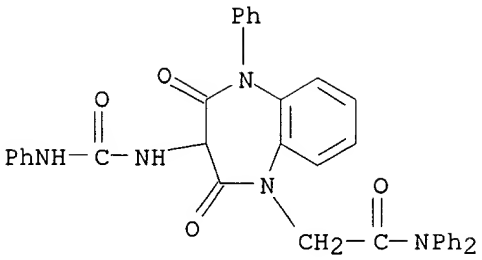
RN 173908-75-3 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



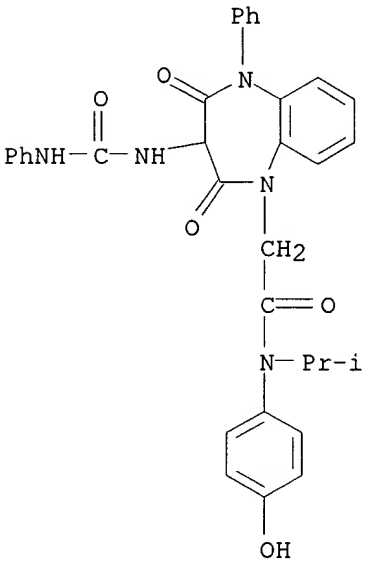
RN 173908-76-4 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-cyclohexyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



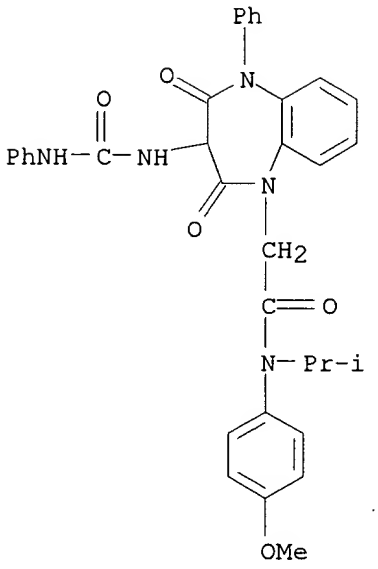
RN 173908-77-5 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,N,5-triphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 173908-78-6 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(4-hydroxyphenyl)-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



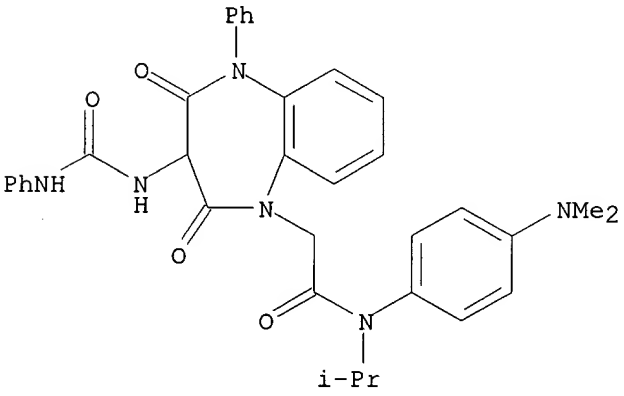
RN 173908-79-7 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(4-methoxyphenyl)-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 173908-81-1 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-[4-(dimethylamino)phenyl]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 161456-17-3
CMF C35 H36 N6 O4



CM 2

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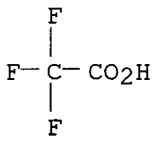
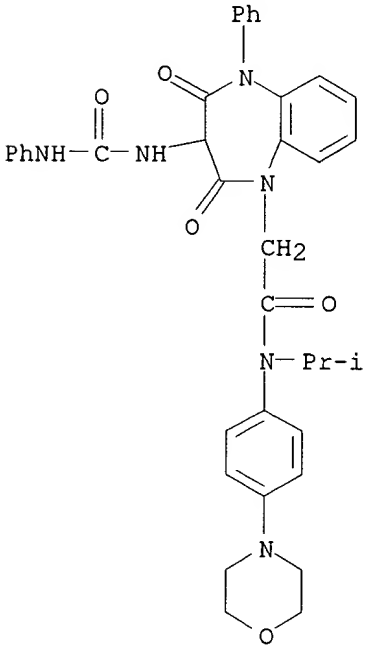
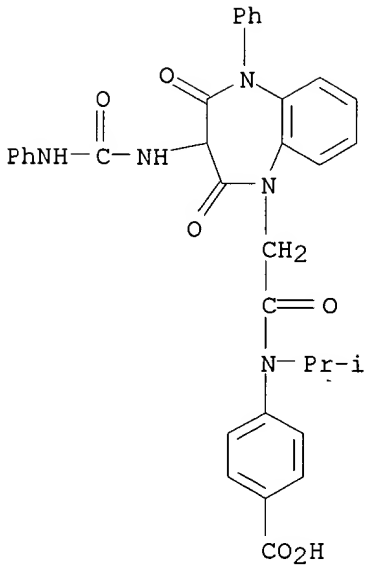
CMF C2 H F3 O2



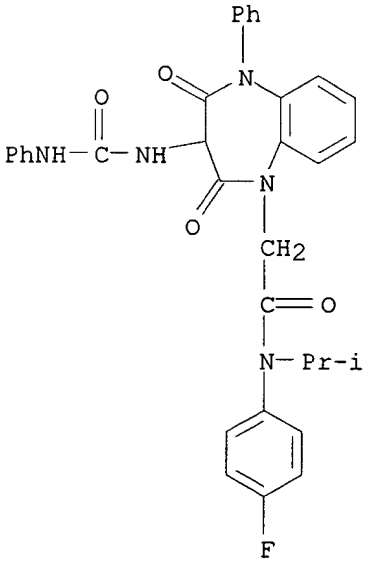
RN 173908-82-2 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-N-[4-(4-morpholinyl)phenyl]-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



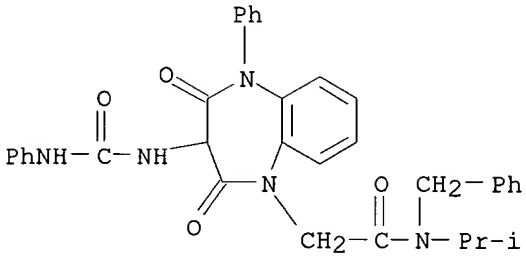
RN 173908-83-3 CAPLUS
CN Benzoic acid, 4-[(1-methylethyl)[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-1H-1,5-benzodiazepin-1-yl]acetyl]amino]- (9CI) (CA INDEX NAME)



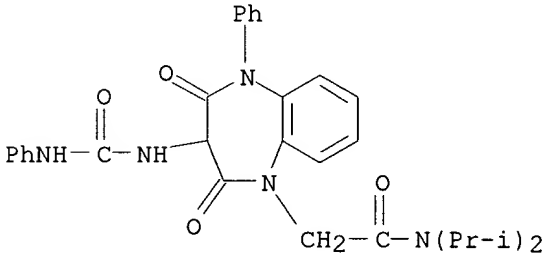
RN 173908-84-4 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-(4-fluorophenyl)-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



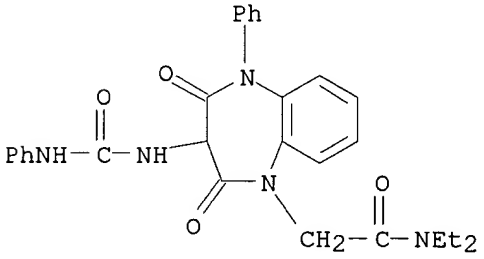
RN 173908-85-5 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



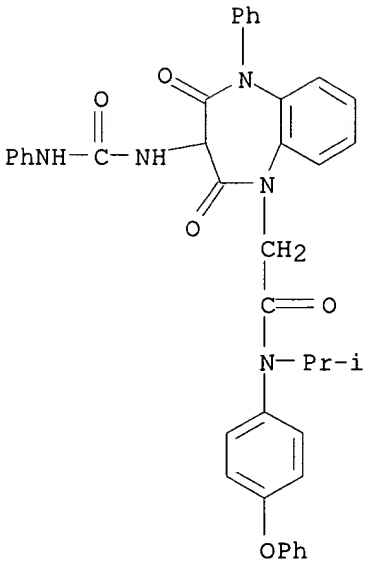
RN 173908-86-6 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N,N-bis(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



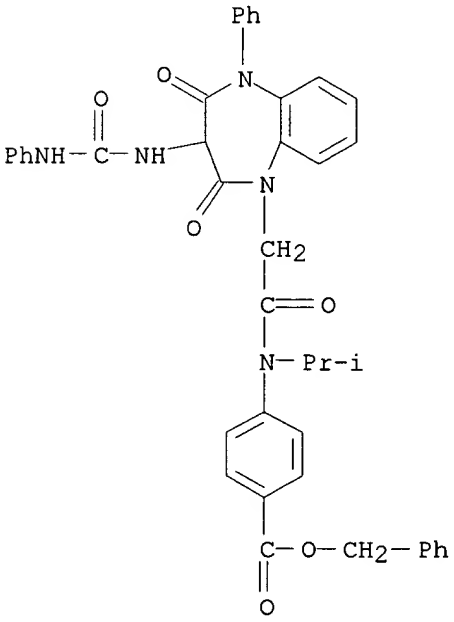
RN 173908-87-7 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N,N-diethyl-2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



IT **173908-92-4 173908-93-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of 1,5-benzodiazepines with peripheral cholecystokinin (CCK-A) agonist activity)
RN 173908-92-4 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N-(4-phenoxyphenyl)-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 173908-93-5 CAPLUS
CN Benzoic acid, 4-[(1-methylethyl)[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-1H-1,5-benzodiazepin-1-yl]acetyl]amino]-, phenylmethyl ester (9CI) (CA INDEX NAME)



L17 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1995:408461 CAPLUS
DN 122:187628
TI Preparation of 1,5-benzodiazepine-2,4-dione derivatives as cholecystokinin A receptor agonists.
IN Sugg, Elizabeth Ellen; Aquino, Christopher Joseph; Szewczyk, Jerzy Ryszard; Finch, Harry; Carr, Robin Arthur Ellis
PA Glaxo Inc., USA
SO PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 9424149 | A1 | 19941027 | WO 1994-EP1131 | 19940414 |
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| | RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
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| | AU 681139 | B2 | 19970821 | | |
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| | ZA 9402571 | A | 19941111 | ZA 1994-2571 | 19940414 |
| | EP 694039 | A1 | 19960131 | EP 1994-913580 | 19940414 |
| | EP 694039 | B1 | 20010124 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE | | | | |
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| | CN 1058487 | B | 20001115 | | |
| | JP 08508744 | T2 | 19960917 | JP 1994-522734 | 19940414 |
| | HU 74102 | A2 | 19961128 | HU 1995-2978 | 19940414 |
| | RU 2135486 | C1 | 19990827 | RU 1995-117974 | 19940414 |
| | CZ 286695 | B6 | 20000614 | CZ 1995-2675 | 19940414 |
| | PL 178790 | B1 | 20000630 | PL 1994-311084 | 19940414 |
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| | US 5646140 | A | 19970708 | US 1995-525659 | 19951013 |
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OS MARPAT 122:187628
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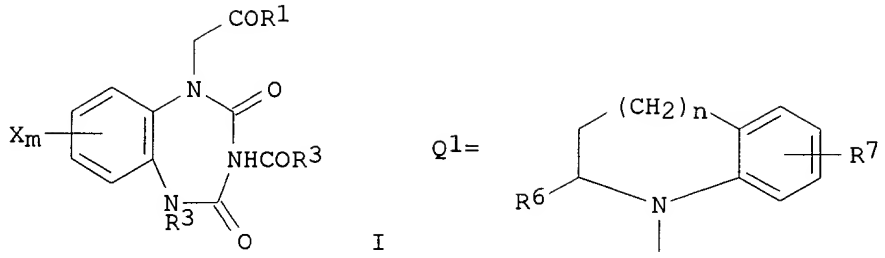
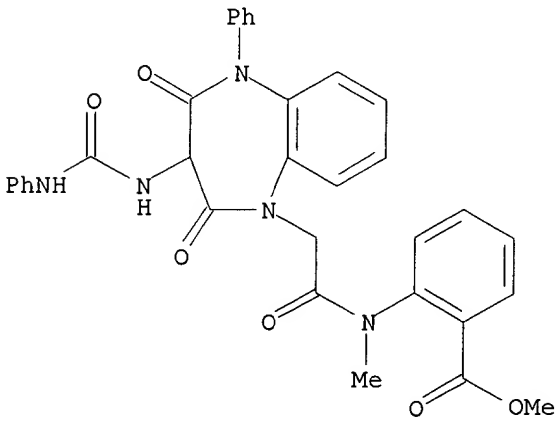


AB Title compds. [I; X = H, CF3, alkyl, alkylthio, alkoxy, halo; R1 = amino, Q1; R2 = (substituted) pyrrolyl, quinolinyl, benzofuryl, benzothienyl, indolyl, indolinyl, Ph, pyridyl, amino, etc.; R3 = H, alkyl, cycloalkyl, (halo)phenyl; R6 = H, Me; R7 = H, OH, F, Me2N, alkoxy, PhCH2O; m, n = 1, 2], were prepd. Thus, 2-(3-amino-2,4-dioxo-5-phenyl-2,3,4,5-tetrahydrobenzo[b][1,4]diazepin-1-yl)-N-isopropyl-N-(4-methoxyphenyl)acetamide (prepn. given) was stirred with indole-2-carboxylic acid, hydroxybenzotriazole, and 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride in DMF to give 1H-indole-2-carboxylic acid [1-[1-isopropyl-(4-methoxyphenyl)carbamoylmethyl]-2,4-dioxo-5-phenyl-2,3,4,5-tetrahydro-1H-benzo[b][1,4]diazepin-3-yl]amide. The latter at 30 .mu.M in a guinea pig gall bladder assay gave 42% contraction relative to acetylcholine at 100%.

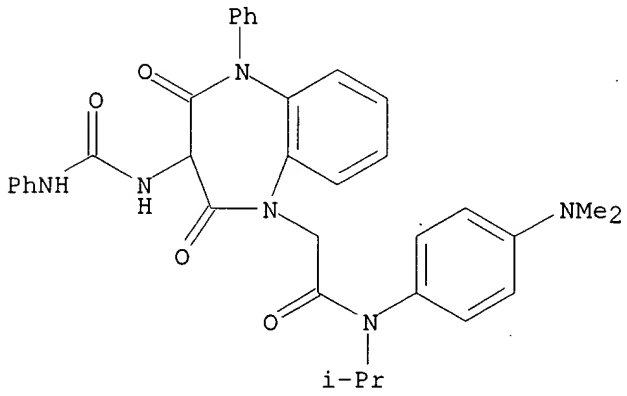
IT **161455-99-8 161456-00-4 161456-01-5 161456-02-6 161456-13-9 161456-14-0 161456-15-1 161456-16-2 161456-17-3 161456-18-4 161456-19-5 161456-20-8 161456-30-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(1,5-benzodiazepine derivs. as cholecystokinin A agonists)

RN 161455-99-8 CAPLUS

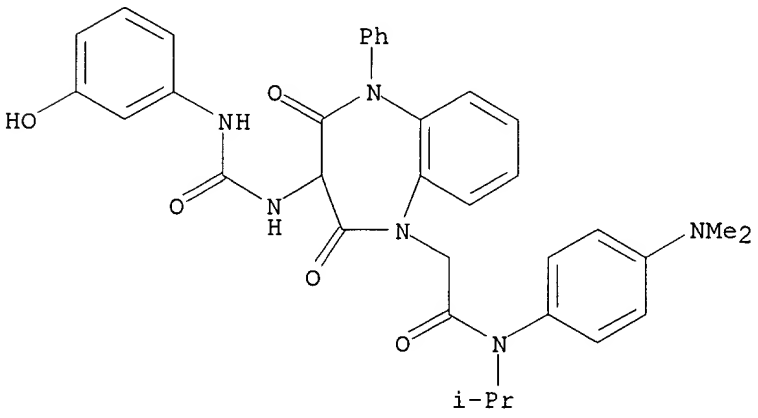
CN Benzoic acid, 2-[methyl[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-1H-1,5-benzodiazepin-1-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



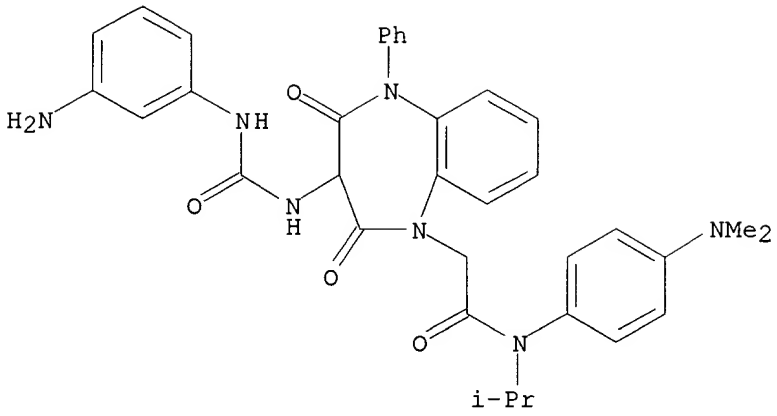
RN 161456-00-4 CAPLUS
RN 161456-01-5 CAPLUS
RN 161456-02-6 CAPLUS
RN 161456-13-9 CAPLUS
RN 161456-14-0 CAPLUS
RN 161456-15-1 CAPLUS
RN 161456-16-2 CAPLUS
RN 161456-17-3 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-[4-(dimethylamino)phenyl]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



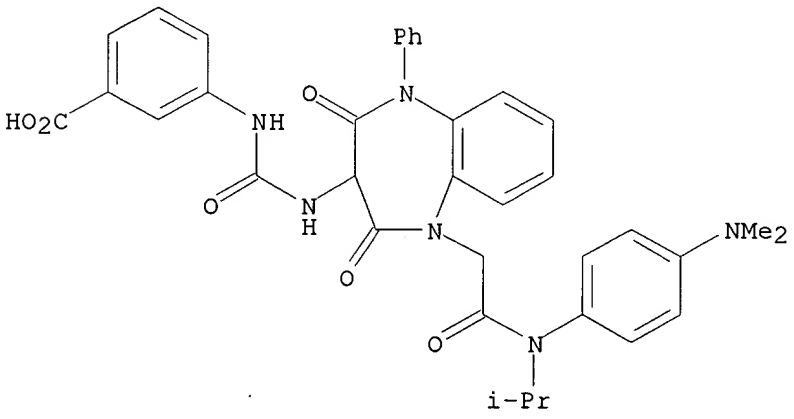

RN 161456-18-4 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-[4-(dimethylamino)phenyl]-2,3,4,5-tetrahydro-3-[[[(3-hydroxyphenyl)amino]carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-5-phenyl- (9CI) (CA INDEX NAME)



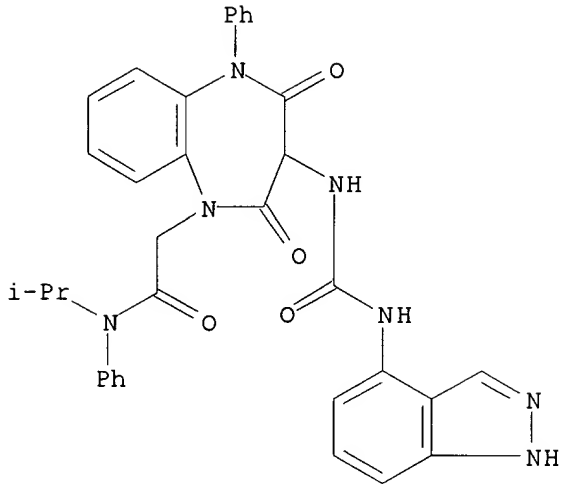

RN 161456-19-5 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-aminophenyl)amino]carbonyl]amino]-N-[4-(dimethylamino)phenyl]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl- (9CI) (CA INDEX NAME)



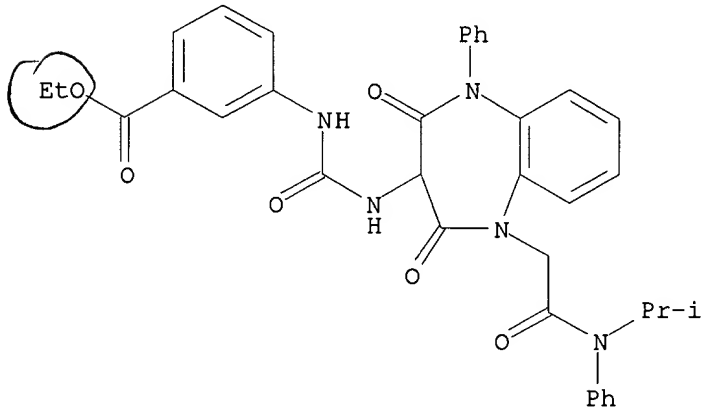
RN 161456-20-8 CAPLUS
CN Benzoic acid, 3-[[[[1-[2-[[4-(dimethylamino)phenyl](1-methylethyl)amino]-2-oxoethyl]-2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 161456-30-0 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-[[(1H-indazol-4-ylamino)carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)

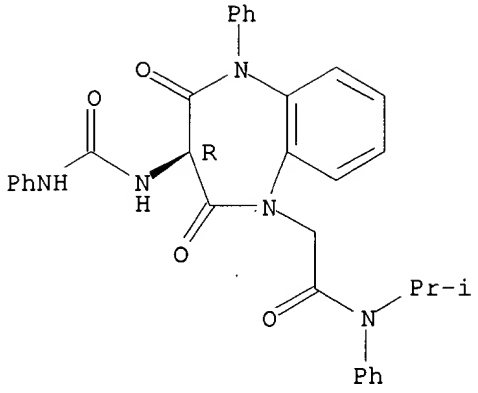


IT **161455-77-2P 161455-81-8P 161455-82-9P**
**161455-83-0P 161513-73-1P 161513-74-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 1,5-benzodiazepine derivs. as cholecystokinin A agonists)
RN 161455-77-2 CAPLUS
RN 161455-81-8 CAPLUS
RN 161455-82-9 CAPLUS
CN Benzoic acid, 3-[[[[2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 161455-83-0 CAPLUS
RN 161513-73-1 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 161513-74-2 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.